

TABLE 1. Continuous Self-Consistent Acidity Scale of Neutral Acids in Acetonitrile

Acid	pK_a (AN) ^a	Directly measured ΔpK_a ^b	Acid	pK_a (AN) ^a	Directly measured ΔpK_a ^b
1 9-C ₉ F ₉ -Fluorene	28.11	1.15	48 3-CF ₃ -C ₆ H ₄ CH(CN) ₂	14.72	0.15
2 (4-Me-C ₆ F ₄)(C ₆ H ₅)CHCN	26.96	0.83 1.98	49 Saccharin	14.57	0.71
3 (4-NC ₆ F ₄)(C ₆ H ₅)NH	26.34	0.20	50 4-Me-C ₆ F ₄ CH(CN) ₂	13.87	0.40
4 (C ₆ H ₅)(C ₆ F ₅)CHCN	26.14	1.03	51 (4-NC ₆ F ₄) ₂ CHCN	13.46	0.45 0.89
5 (4-Me ₂ N-C ₆ F ₄)(C ₆ F ₅)NH	25.12	1.20	52 C ₆ F ₅ CH(CN) ₂	13.01	0.03
6 (4-Me-C ₆ F ₄)(C ₆ F ₅)NH	24.94	0.64	53 4-H-C ₆ F ₄ CH(CN) ₂	12.98	0.74
7 Octafluorofluorene	24.49	0.45	54 2-C ₁₀ F ₇ CH(CN) ₂	12.23	1.38 0.26
8 Fluoradene	23.90	0.96	55 Tos ₂ NH ^c	11.97	0.62
9 9-COO ⁻ Me-Fluorene	23.53	1.05 -0.01	56 4-NO ₂ -C ₆ H ₄ CH(CN) ₂	11.61	0.63
10 Acetic acid	23.51	0.67	57 4-MeO-C ₆ H ₄ C(=O)NHTf ^d	11.60	0.28
11 (C ₆ F ₅)CH(COOEt) ₂	22.85	0.73	58 4-Me-C ₆ H ₄ C(=O)NHTf	11.46	0.98
12 2-NO ₂ -Phenol	22.85	0.92	59 (C ₆ H ₅ SO ₂) ₂ NH	11.34	0.60
13 (4-Me-C ₆ F ₄) ₂ CHCN	22.80	0.90	60 4-Cl-C ₆ H ₄ SO ₂ NHTos	11.10	0.36
14 (4-Me-C ₆ F ₄)(C ₆ F ₅)CHCN	21.94	0.42	61 C ₆ H ₄ C(=O)NHTf	11.06	1.43
15 Benzoic acid	21.51	0.60	62 Picric acid	11.00	0.57
16 9-CN-Fluorene	21.36	0.39 0.25	63 4-F-C ₆ H ₄ C(=O)NHTf	10.65	0.78
17 (4-H-C ₆ F ₄)(C ₆ F ₅)CHCN	21.11	0.26	64 4-Cl-C ₆ H ₄ C(=O)NHTf	10.36	0.82
18 (C ₆ F ₅) ₂ CHCN	21.10	1.01	65 4-Cl-C ₆ H ₄ SO ₂ ₂ NH	10.20	0.15
19 (CF ₃) ₂ COH	20.55	0.76	66 4-CF ₃ -C ₆ F ₄ CH(CN) ₂	10.19	0.14
20 (4-Cl-C ₆ F ₄)(C ₆ F ₅)CHCN	20.36	0.53	67 4-NO ₂ -C ₆ H ₄ SO ₂ NHTos	10.04	0.52
21 2,4,6-Br ₃ -Phenol	20.35	1.02	68 4-Cl-3-NO ₂ -C ₆ H ₄ SO ₂ NHTos	9.71	1.05
22 (2,4,6-Cl ₃ -C ₆ F ₃)(C ₆ F ₅)CHCN	20.13	0.21	69 4-NO ₂ -C ₆ H ₄ C(=O)NHTf	9.49	0.53
23 2,3,5,6-F ₄ -Phenol	20.12	0.03	70 4-NO ₂ -C ₆ H ₄ SO ₂ NHSO ₂ -C ₆ H ₄ -4-Cl	9.17	0.56 1.73
24 2,3,4,5,6-F ₅ -Phenol	20.11	0.42	71 TosOH	8.6	1.21 0.23
25 (2-C ₆ F ₇)(C ₆ F ₅)CHCN	20.08	0.01	72 (4-NO ₂ -C ₆ H ₄ SO ₂) ₂ NH	8.32	1.3
26 1-C ₆ F ₇ OH	19.72	0.43	73 1-C ₁₀ H ₇ SO ₃ H	8.02	0.19 0.04
27 2,4,6-(SO ₂ F) ₂ -Aniline	19.66	0.40	74 C ₆ H ₅ CHTf ₂	7.85	0.54 1.25
28 (2-C ₆ F ₇) ₂ CHCN	19.32	0.34	75 4-Cl-C ₆ H ₄ SO ₃ H	7.3	0.53
29 9-C ₉ F ₉ -Octafluorofluorene	18.86	0.38 1.19	76 3-NO ₂ -C ₆ H ₄ SO ₃ H	6.78	0.51
30 2-C ₁₀ F ₇ OH	18.50	0.36	77 4-NO ₂ -C ₆ H ₄ SO ₃ H	6.73	0.51
31 (4-CF ₃ -C ₆ F ₄)(C ₆ F ₅)CHCN	18.14	0.48	78 4-MeO-C ₆ H ₄ C(=O)NHTf	6.54	0.51
32 4-C ₆ F ₅ -2,3,5,6-F ₄ -Phenol	18.11	0.06	79 4-Me-C ₆ H ₄ C(=O)NHTf	6.32	0.44
33 (4-H-C ₆ F ₄)CH(CN)COOEt	18.08	0.46	80 TosNHTf	6.30	0.75
34 2,3,4,5,6-Cl ₅ -Phenol	18.02	0.19	81 C ₆ H ₄ C(=O)NHTf	6.17	0.36
35 2,3,4,5,6-Br ₅ -Phenol	17.83	0.59	82 C ₆ H ₅ SO ₂ NHTf	6.02	0.59
36 (C ₆ F ₅)CH(CN)COOEt	17.75	0.09	83 4-F-C ₆ H ₄ C(=O)NHTf	5.79	0.83
37 4-Me-C ₆ H ₄ CH(CN) ₂	17.59	1.15	84 4-Cl-C ₆ H ₄ C(=O)NHTf	5.69	0.77
38 (2-C ₆ F ₇)CH(CN)COOEt	17.50	1.10	85 2,4,6-(SO ₂ F) ₃ -Phenol	5.66	0.77
39 (4-Cl-C ₆ F ₄)CH(CN)COOEt	17.39	0.32 0.10	86 4-Cl-C ₆ H ₄ SO ₂ NHTf	5.47	0.71
40 2,4-(NO ₂) ₂ -Phenol	16.66	0.77	87 4-Cl-C ₆ H ₄ SO(=O)NHTos	5.27	0.53
41 4-CF ₃ -2,3,5,6-F ₄ -Phenol	16.62	1.49 0.22	88 4-NO ₂ -C ₆ H ₄ C(=O)NHTf	5.13	0.38
42 (4-NC ₆ F ₄)(C ₆ F ₅)CHCN	16.40	0.60	89 2,4,6-Tf ₃ -Phenol	4.93	0.41
43 (4-CF ₃ -C ₆ F ₄) ₂ CHCN	16.13	0.32	90 4-NO ₂ -C ₆ H ₄ SO ₂ NHTf	4.52	0.65
44 (4-CF ₃ -C ₆ F ₄)CH(CN)COOEt	16.08	0.08	91 4-Cl-C ₆ H ₄ SO(=O)NHTf	4.47	0.31
45 (4-NC ₆ F ₄)(2-C ₆ F ₇)CHCN	16.02	1.32	92 2,3,5-tricyanocyclopentadiene	4.16	0.50
46 4-NC ₆ F ₄ -OH	15.40	1.12 1.35	93 4-Cl-C ₆ H ₄ SO(=O)NHTf	3.75	1.10 1.15
47 (4-NC ₆ F ₄)CH(CN)COOEt	14.90	0.19			

^a Absolute pK_a values (see the Results). ^b The numbers on the arrows are the experimental ΔpK_a values from this work and previous works.^{6,20} ^c Tos denotes 4-Me-C₆H₄SO₂-. ^d Tf denotes CF₃SO₂-.